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Molecular beam epitaxy of β-$FeSi_2$ films on Si(111) substrates and its influence on minority-carrier diffusion length of Si measured by EBIC

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Abstract

We have studied the influence of molecular beam epitaxy (MBE) of β-$FeSi_2$ films on minority-carrier diffusion length of an n-type Si(111) substrate. It was found from electron beam induced current technique that the diffusion length was less influenced in sample formed with a β-$FeSi_2$ template prior to the MBE growth than that in sample grown without the template. The size of β-$FeSi_2$ grains measured by electron back-scatter diffraction was also discussed.

Keywords: β-$FeSi_2$; EBIC; EBSD; minority carrier dissusion length

1. Introduction

We have been paying special attention to semiconducting β-$FeSi_2$ as a promising material for use in silicon-based light emitters and detectors operating at a wavelength of approximately 1.5 µm [1-3]. This material has a large absorption coefficient of over 10^5 cm^{-1} at 1 eV [4], and it can be grown epitaxially on Si substrates. Therefore, the formation of a *p*/*n* junction using the β-$FeSi_2$/Si heterostructure has been studied extensively for the application of various kinds of β-$FeSi_2$ devices on Si substrates. In the past twenty years, a number of growth methods have been attempted for the formation of β-$FeSi_2$ films. However, the β-$FeSi_2$ films are composed of epitaxial variants in most cases, because the lattice constant *b* is very close to *c* [5]. Another puzzling problem in the β-$FeSi_2$/Si heterostructure is the diffusion of Fe atoms into the Si substrate near the interface. Liu *et al*. investigated the effect of β-$FeSi_2$ template on the depth profiles of Fe atoms in the Si substrate by Auger electron spectroscopy [6]. They prepared β-$FeSi_2$ films by molecular beam epitaxy (MBE) with and without the β-$FeSi_2$ template prior to the MBE

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growth. The influence of high temperature annealing (880˚C for 2 h) was also examined. It was found that the template reduced the Fe diffusion into the Si substrate, and also that the Fe diffusion was effectively hindered by the template even after the annealing was performed. Diffused Fe atoms are known to form deep levels in Si, and thus they are supposed to work as efficient traps for minority carriers [7,8]. However, there have been no reports to date on the influence of β-$FeSi_2$ formation on minority-carrier diffusion length of Si, which is one of the most decisive parameters limiting the device performance. Therefore, it is of great importance to evaluate this influence.

The purpose of the present work is to form β-$FeSi_2$ films by MBE on an n-type Si(111) substrate, and to investigate its influence on the minority carrier diffusion length in the Si.

2. Experiment

N-type Czochralski Si(111) substrates with resistivity of 0.5-0.7 Ω·cm were used. The substrate was cleaned and thin protective oxide layer was formed by the RCA method. We prepared two kinds of samples A and B. For sample A, an approximately 20-nm-thick highly [110]/[101]-oriented β-$FeSi_2$ epitaxial template was formed at 650 °C by reactive deposition epitaxy (RDE), that is Fe deposition on a hot Si substrate. Then, Fe and Si were coevaporated on the template at 750 °C to form β-$FeSi_2$ continuous films by MBE [9]. For sample B, Fe and Si were directly coevaporated on the Si substrate by MBE. After the MBE growth of β-$FeSi_2$ layers in both samples, β-$FeSi_2$ layers were etched away with a diluted HF acid (50%) for 30 min, and then the Schottky contact was formed with Au at the surface side. Ohmic contact was formed with Al on the back side.

The crystalline quality of the grown layers was characterized by x-ray diffraction (XRD). The observation of microstructure was carried out by scanning electron microscopy (SEM).The grain size of β-$FeSi_2$ was evaluated using EBSD. The minority carrier diffusion length was measured by electron beam induced current (EBIC) technique.

3. Results and discussion

Figures 1(a) and 1(b) show the θ–2θ XRD patterns for sample A, prepared with the template, and sample B, prepared without the template, respectively. In the XRD pattern of sample A, intense peaks of (220)/(202) and (440)/(404) of β-$FeSi_2$ were clearly seen near the (111) and (222) peaks of the Si substrate, respectively. Thus, highly [110] and/or [101]-oriented β-$FeSi_2$, matching the epitaxial relationship of β-$FeSi_2$ on Si(111), was formed in sample A. On the other hand, the diffraction peaks from various planes exist in sample B, showing that β-$FeSi_2$ in sample B was polycrystalline.

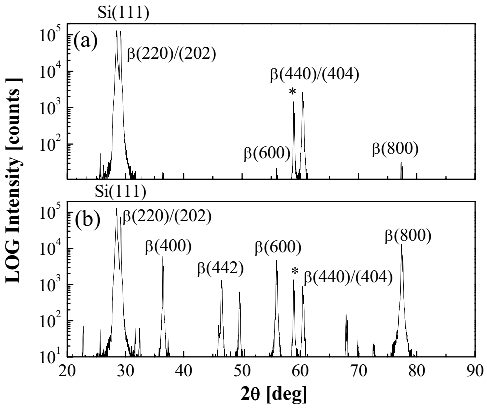

Fig.1 θ-2θ XRD pattern of (a) sample A and (b) sample B.

Figures 2(a) and 2(b) show the EBSD mappings of β-$FeSi_2$ for samples A and B, respectively, observed along the normal directions. The area of (110)-oriented β-$FeSi_2$ grains is colored blue, while (101)-oriented β-$FeSi_2$ grains is colored yellow, and that of the (100)-oriented β-$FeSi_2$ grains is colored green. The grain size of β-$FeSi_2$ is estimated to be a few μm in both samples. However, there exists a clear difference in crystal orientation of β-$FeSi_2$ between them. Figure 2(a) reveals that most of the β-$FeSi_2$ grains were formed with [110]/[101] orientation due to the template layer, matching the epitaxial relation to the Si (111) substrate. On the contrary, approximately 80% of β-$FeSi_2$ grains were colored green in sample B, meaning that [100]-oriented β-$FeSi_2$ were formed.

Figure 3(a) show the EBIC image taken around the Au/n-Si Schottky contact formed on the n-Si substrate (sample C). On the other hand, Figs. 3(b) and 3(c) are EBIC images of Au/n-Si Schottky contacts, which were formed after the β-$FeSi_2$ layers were etched away from the surfaces in samples A and B, respectively. We denote these samples A' and B', respectively, hereafter. The acceleration voltage of electron beam was 10 kV. In the EBIC measurement, the carriers generated within a diffusion length from the depletion edge on the n-type Si are collected by the electric field under the Au contact and sensed as a current in the external circuit. As shown in Fig. 3, the brighter regions indicate higher collection of electron-beam-induced carriers in Si. The EBIC decreased gradually away from the edge of the electrode. In Fig. 3(b), there are many dark spots observed in the contact region. In sample A', many island-like structures were observed by AFM after the etching. Thus, we think that the dark spots indicate a rough surface of sample A'.

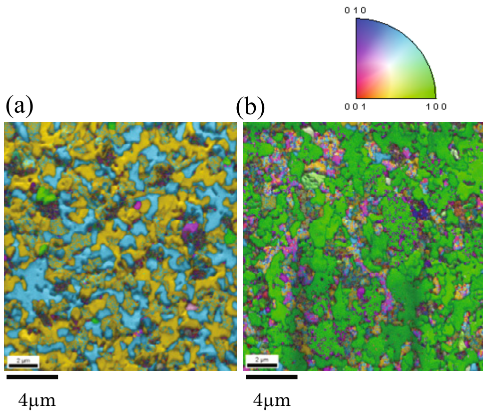

Fig. 2 EBSD mappings of β-$FeSi_2$ observed along normal direction for (a) sample A, grown with the template layer, and (b) sample B, grown without the template layer.

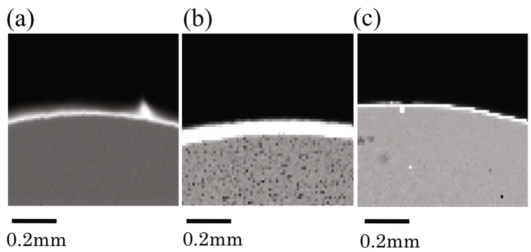

Fig. 3 EBIC images around the Au/n-Si Schottky contact for (a) sample C, (b) sample A' and (c) sample B'.

Figure 4 shows the semi logarithmic plots of EBIC line-scan data. The EBIC profiles show a clear exponential dependence of distance from the Au contact. Several theoretical models have been used to extract the minority carrier diffusion length by fitting the theoretical expression to the EBIC line-scan date. The EBIC profile varies as $\exp(-x/L)$, where x is the distance from the Au edge, and L the diffusion length of holes. In this work, the diffusion lengths were estimated to be 23 μm for the single-crystalline Si, 16 μm for the sample grown with template, and 3 μm for the sample grown without template. On the basis of these results, it can be at least concluded that β-$FeSi_2$ template reduces the Fe diffusion into the Si substrate during the β-$FeSi_2$ film fabrication, thereby preventing the decrease in minority-carrier diffusion length in the Si.

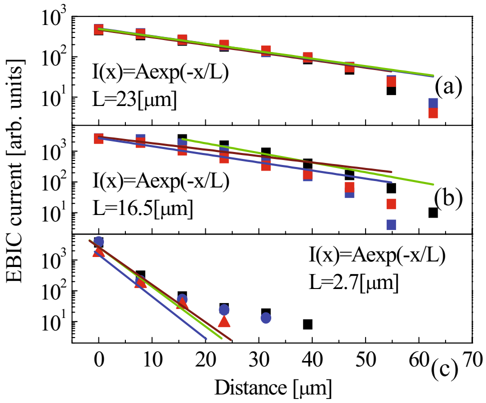

Fig. 4 Semilogarithmic plots of EBIC line-scan profiles measured at room temperature on (a) sample C, (b) sample A', and (c) sample B'.

4. Conclusions

We have formed β-$FeSi_2$ films by MBE on an n-type Si(111) substrate, and to investigate its influence on the minority carrier diffusion length in the Si after the β-$FeSi_2$ films were etched away and the Au/n-Si Schottky contact was formed on the n-Si substrate. It was found from the EBIC measurements that the diffusion length of holes in n-Si was drastically decreased down to 3 μm for the n-Si substrate on which the β-$FeSi_2$ films were formed without the template. This value is much smaller than 16 μm for the n-Si on which the β-$FeSi_2$ films were formed with the template, and 23 μm for the non-processed n-Si substrate.

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References

[1] T. Suemasu, Y. Negishi, K. Takakura and F. Hasegawa, Jpn. J. Appl. Phys., Part 2 **39**3 (2000) L1013.
[2] T. Ootsuka, Y. Fudamoto, M. Osamura, T. Suemasu, Y. Makita, Y. Fukuzawa and Y. Nakayama, Appl. Phys. Lett. **91** (2007) 142114.
[3] M. Suzuno, T. Koizumi and T. Suemasu, Appl. Phys. Lett. **94** (2009) 213509.
[4] M. C. Bost and John E. Mahan, J. Appl. Phys. **64** (1998) 2034.
[5] T. Kimura, K. Akiyama, T. Watanabe, K. Saito and H. Funakubo, Jpn. J. Appl. Phys. **42** (2003) 4943.
[6] Z. Liu, Y. Suzuki, M. Osamura, T. Ootsuka, T. Mise, R. Kuroda, H. Tanoue, Y. Makita, S. Wang, Y. Fukuzawa, N. Otogawa and Y. Nakayama, J. Appl. Phys. **95** (2004) 4019.
[7] K. Wünstel and P. Wagner, Appl. Phys. A: Solids Surf. **27** (1982) 207.
[8] T. Isobe, H. Nakashima and K. Hashimoto, Jpn. J. Appl. Phys., Part 1 **28** (1989) 1282.
[9] M. Takauji, N. Seki, T. Suemasu, F. Hasegawa and M. Ichida, J. Appl. Phys. **65** (2004) 2561.